Ground-state properties of the spin-1/2 Heisenberg-Ising bond alternating chain with Dzyaloshinskii-Moriya interaction

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Abstract

Ground-state energy is exactly calculated for the spin-1/2 Heisenberg-Ising bond alternating chain with the Dzyaloshinskii-Moriya interaction. Under certain condition, which relates a strength of the Ising, Heisenberg and Dzyaloshinskii-Moriya interactions, the ground-state energy exhibits an interesting nonanalytic behavior accompanied with a gapless excitation spectrum.

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Quantum spin chains provide an excellent playground for theoretical studies of collective quantum phenomena as they may exhibit numerous exotic ground states and quantum critical points [1]. The spin-1/2 Heisenberg-Ising bond alternating chain, which has been originally invented by Lieb *et al.* [2] and recently re-examined by Yao *et al.* [3], represents a valuable example of rigorously solved quantum spin chain. The present work aims to provide a generalization of this simple but nontrivial quantum spin model by taking into account the antisymmetric Dzyaloshinskii-Moriya interaction.

Let us consider a bond alternating chain of $2N$ spins 1/2 with nearest-neighbor antiferromagnetic interactions, which are alternatively of the Heisenberg and Ising type, respectively. The total Hamiltonian of the model under consideration is given by

$$\begin{aligned} H = \sum_{n=1}^{N} \Big[& J_{\rm H} (s_{2n-1}^x s_{2n}^x + s_{2n-1}^y s_{2n}^y + \Delta s_{2n-1}^z s_{2n}^z) \\ & + D \left(s_{2n-1}^x s_{2n}^y - s_{2n-1}^y s_{2n}^x \right) + 2 J_{\rm I} s_{2n}^z s_{2n+1}^z \Big], \end{aligned} \tag{1}$$

where the parameter $J_{\rm H}(\Delta)$ denotes the XXZ Heisenberg interaction between $2n-1$ and $2n$ spins, Δ is an anisotropy in this interaction, and the parameter D stands for the z component of the antisymmetric Dzyaloshinskii-Moriya interaction present along the Heisenberg bonds. Furthermore, the term $2J_{\rm I}$ denotes the Ising interaction between $2n$ and $2n+1$ spins and the periodic boundary condition $s_{2N+1}^{\alpha} \equiv s_1^{\alpha}$ $(\alpha = x, y, z)$ is imposed for convenience.

First, let us eliminate from the Hamiltonian (1) the Dzyaloshinskii-Moriya term after performing a spin coordinate transformation. The spin rotation about the z-axis by the specific angle $\tan\varphi = D/J_{\rm H}$, which is performed at all even sites $2n$ $(n = 1, \ldots, N)$,

$$s_{2n}^x \to s_{2n}^x \cos\varphi + s_{2n}^y \sin\varphi, \;\; s_{2n}^y \to -s_{2n}^x \sin\varphi + s_{2n}^y \cos\varphi,$$

ensures a precise mapping equivalence between the Hamiltonian (1) and the Hamiltonian

$$\begin{aligned} H = \sum_{n=1}^{N} \Big[& \sqrt{J_{\rm H}^2 + D^2} \left(s_{2n-1}^x s_{2n}^x + s_{2n-1}^y s_{2n}^y \right) \\ & + J_{\rm H} \Delta s_{2n-1}^z s_{2n}^z + 2 J_{\rm I} s_{2n}^z s_{2n+1}^z \Big]. \end{aligned} \tag{2}$$

From here onward, one may closely follow the rigorous procedure developed in Refs. [2, 3]. According to this, the Hamiltonian (2) is rewritten in terms of raising and lowering operators in the subspace where the ground state is, and subsequently, the Jordan-Wigner transformation is applied to express the relevant spin Hamiltonian as a bilinear form of Fermi

operators. The Fourier and Bogolyubov transformations are finally employed to bring the Hamiltonian relevant for the ground-state properties into the diagonal form

$$H = -\frac{N}{4} J_{\rm H} \Delta + \sum_k \Lambda_k \left(\beta_k^{\dagger} \beta_k - \frac{1}{2} \right), \tag{3}$$

where

$$\Lambda_k = \sqrt{\left(\sqrt{J_{\rm H}^2 + D^2} + J_{\rm I} \right)^2 - 4 \sqrt{J_{\rm H}^2 + D^2} J_{\rm I} \cos^2 \frac{k}{2}}. \tag{4}$$

From Eqs. (3) and (4) one easily finds the exact result for the ground-state energy of the antiferromagnetic spin-1/2 Heisenberg-Ising bond alternating chain (1) for $N \to \infty$

$$\frac{E_0}{N} = -\frac{1}{4} J_{\rm H} \Delta - \frac{\sqrt{J_{\rm H}^2 + D^2} + J_{\rm I}}{\pi} {\rm E}(a), \tag{5}$$

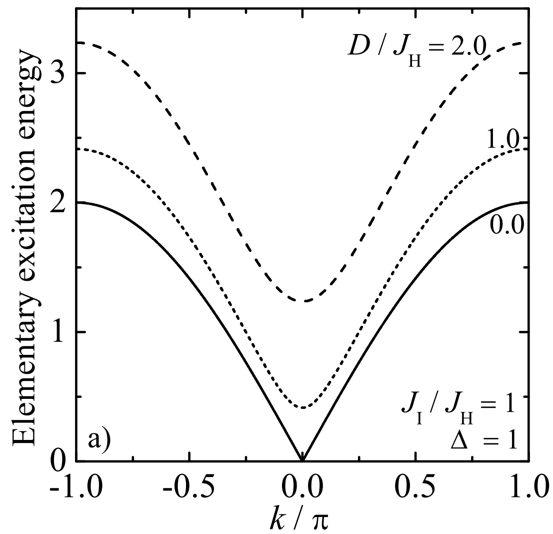
where ${\rm E}(a) = \int_0^{\frac{\pi}{2}} {\rm d}\theta \sqrt{1 - a^2 \sin^2 \theta}$ is the complete elliptic integral of the second kind with the modulus a,

$$a^2 = \frac{4 \sqrt{J_{\rm H}^2 + D^2} J_{\rm I}}{\left(\sqrt{J_{\rm H}^2 + D^2} + J_{\rm I} \right)^2} \geq 0.$$

Recall that the complete elliptic integral of the second kind is a nonanalytic function of its modulus for $a^2 = 1 - (a')^2 \approx 1$, i.e., ${\rm E}(a) - 1 \propto \ln a' (a')^2$. The condition $a^2 = 1$ holds just if $J_{\rm I} = \sqrt{J_{\rm H}^2 + D^2}$ and hence, one may expect nonanalytic behavior of the ground-state energy (5) under this special constraint, which relates a strength of the Ising, Heisenberg and Dzyaloshinskii-Moriya interactions.

Before proceeding to a more detailed discussion of the most interesting results, it is worthy to mention that our exact results correctly reproduce (in an absence of the Dzyaloshinskii-Moriya term) the results previously reported by Lieb *et al.* [2] for the isotropic version and by Yao *et al.* [3] for the anisotropic version of the antiferromagnetic spin-1/2 Heisenberg-Ising bond alternating chain. For simplicity, our subsequent analysis will be restricted just to a particular case of the model with the isotropic Heisenberg interaction ($\Delta = 1$), which exhibits all general features notwithstanding this limitation.

In Fig. 1 we depict the elementary excitation energy spectrum Λ_k calculated from Eq. (4) for two different values of the ratio $J_{\rm I}/J_{\rm H}$ and several values of the Dzyaloshinskii-Moriya anisotropy $D/J_{\rm H}$. Generally, the excitations are gapped with exception of the particular cases that satisfy the condition $J_{\rm I} = \sqrt{J_{\rm H}^2 + D^2}$. The gapless excitation spectrum might be



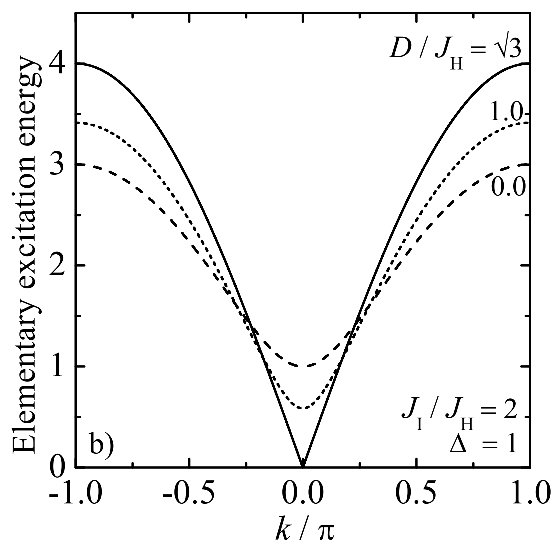


FIG. 1: Elementary excitation spectrum for several values of the Dzyaloshinskii-Moriya term D/J_{H}, $\Delta = 1$ and two different values of the ratio: a) $J_{\mathrm{I}}/J_{\mathrm{H}} = 1$; b) $J_{\mathrm{I}}/J_{\mathrm{H}} = 2$.

consequently found just if $J_{\mathrm{I}}/J_{\mathrm{H}} \geq 1$, which means that the Ising interaction must be at least twice as large as the Heisenberg one. If $D/J_{\mathrm{H}} = 0$ is assumed, the system has gapless excitation spectrum for $J_{\mathrm{I}}/J_{\mathrm{H}} = 1$ in accordance with the previously published results [2, 3]. Interestingly, the gapless excitation spectrum emerges at higher values of the ratio $J_{\mathrm{I}}/J_{\mathrm{H}}$ regardless of the exchange anisotropy Δ whenever the Dzyaloshinskii-Moriya anisotropy is raised from zero.

The three-dimensional plot of the ground-state energy (5) is depicted in Fig. 2 as a

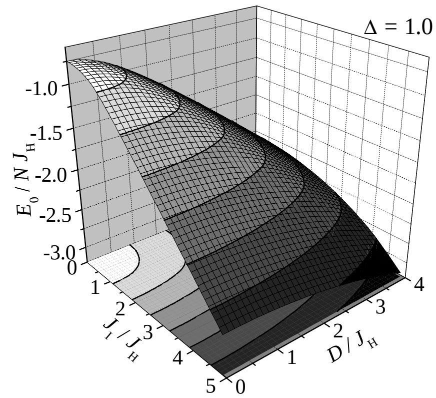


FIG. 2: Ground-state energy as a function of the Dzyaloshinskii-Moriya anisotropy $D/J_{\rm H}$ and the interaction ratio $J_{\rm I}/J_{\rm H}$ for the anisotropy parameter $\Delta = 1$.

function of the ratio $J_{\rm I}/J_{\rm H}$ between the Ising and Heisenberg interaction, as well as, a relative strength of the Dzyaloshinskii-Moriya anisotropy $D/J_{\rm H}$. Referring to this plot, the ground-state energy monotonically decreases upon strengthening the ratio $J_{\rm I}/J_{\rm H}$ and/or the Dzyaloshinskii-Moriya term $D/J_{\rm H}$. In accordance with this statement, the ground-state energy $E_0/NJ_{\rm H} = -3/4$ of a system of the isolated Heisenberg dimers, which is achieved in the limit $J_{\rm I}/J_{\rm H} \to 0$ and $D/J_{\rm H} \to 0$, represents an upper bound for the ground-state energy. Within the manifold $J_{\rm I} = \sqrt{J_{\rm H}^2 + D^2}$, the ground-state energy exhibits a rather striking nonanalytic behavior. Although this weak nonanalytic behavior cannot be seen from Fig. 2, it should manifest itself in higher derivatives of the ground-state energy.

In the present work, the ground-state properties of the spin-1/2 Heisenberg-Ising bond alternating chain with the Dzyaloshinskii-Moriya interaction have been investigated using a series of exact (rotation, Jordan-Wigner, Fourier, Bogolyubov) transformations. Exact results for the ground-state energy and elementary excitation spectrum have been examined in relation with a strength of the ratio between the Ising and Heisenberg interaction, as well as, the Dzyaloshinskii-Moriya term. The most interesting finding to emerge from our study closely relates to a remarkable nonanalytic behavior of the ground-state energy, which is accompanied with the gapless excitation spectrum whenever the condition $J_{\rm I} = \sqrt{J_{\rm H}^2 + D^2}$ is met.

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